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Compilation, Curation, and Meta-Analysis of Kinetic Data on the Reduction of Contaminants by Natural and Engineered Materials

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Contaminants are subject to a variety of abiotic transformation reactions in the environment, including hydrolysis, photolysis, oxidation, and reduction. Abiotic reduction of organic contaminants mostly involves dehalogenation and nitro reduction, and reduction is a major factor in the fate of metal(loid) oxyanions, but there is a wide range of other less-prominent examples. Most of these transformations involve electron-transfer from ferrous iron or sulfide, but the specific donor can range from dissolved-complexed Fe(II) to nano Fe(0). The kinetics of these reactions have been studied extensively to understand their role in natural attenuation and remediation of contaminants. Most of these studies report pseudo-first-order observed rate constants, and those involving heterogeneous reductants usually report mass- and/or surface-area normalized rate constants. These rate constants often are subject to (correlation) analysis and modeling within the dataset from an individual study, or across a few studies of limited scope (e.g., dechlorination by zerovalent iron). However, more comprehensive analyses of these data (e.g., by machine learning methods) is limited by the many practical and fundamental challenges that arise when compiling and curating data from many diverse sources. We have been working to overcome these challenges through the compilation of a database that includes a large portion of the currently published kinetic data and their associated meta-data. We plan to publish the first version of the Abiotic Reduction Kinetics (ARK) database at zenodo.org in Spring 2025. Currently, ARK includes over 4000 rate constants for ~150 contaminants from ~200 publications, with +100 types of meta-data that define the reaction conditions. There are many aspects of the process and results of assembling such a database that can be used to illuminate fundamental issues related to abiotic contaminant transformation under environmental conditions. One prominent example is the harmonization of rate constant representations to allow comparisons across systems without undue loss of precision. Another example is characterization of reducing systems (e.g. fresh vs. aged minerals ± Fe(II)aq) in ways that efficiently represent rate controlling factors. Advances on both these fronts are needed to enable correlation analysis—and ultimately quantitative structure-reactivity relationships—that describe this whole domain of reactivity.